

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
 Data File : BP007099.D
 Acq On : 22 Sep 2021 15:45
 Operator : CG/JU
 Sample : M3804-01 10X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CL-01-091721

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007099.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.899	811	818	828	rBV	1187977	1881404	2.65%	1.007%
2	10.699	1285	1294	1303	rBV	1601365	2661267	3.75%	1.425%
3	14.528	1939	1945	1951	rBV	2426902	3462251	4.87%	1.854%
4	17.275	2407	2412	2418	rBV	2763800	3915996	5.51%	2.097%
5	17.951	2522	2527	2532	rBV	811350	1100808	1.55%	0.589%
6	18.222	2555	2573	2591	rBV2	18377888	71052745	100.00%	38.048%
7	18.622	2637	2641	2646	rVB	729240	941497	1.33%	0.504%
8	19.210	2737	2741	2745	rBV	1776350	2224224	3.13%	1.191%
9	19.269	2746	2751	2753	rBV	2856779	4403469	6.20%	2.358%
10	19.445	2767	2781	2796	rVB	19319355	60201938	84.73%	32.237%
11	19.834	2844	2847	2862	rVB2	950075	1552799	2.19%	0.831%
12	20.710	2986	2996	3017	rVB3	3726106	14961948	21.06%	8.012%
13	21.086	3056	3060	3064	rBV	857877	1497812	2.11%	0.802%
14	21.139	3065	3069	3085	rVB2	3212344	7200770	10.13%	3.856%
15	21.363	3102	3107	3111	rBV	3441206	4605814	6.48%	2.466%
16	23.780	3512	3518	3535	rVB2	2400507	5082175	7.15%	2.721%

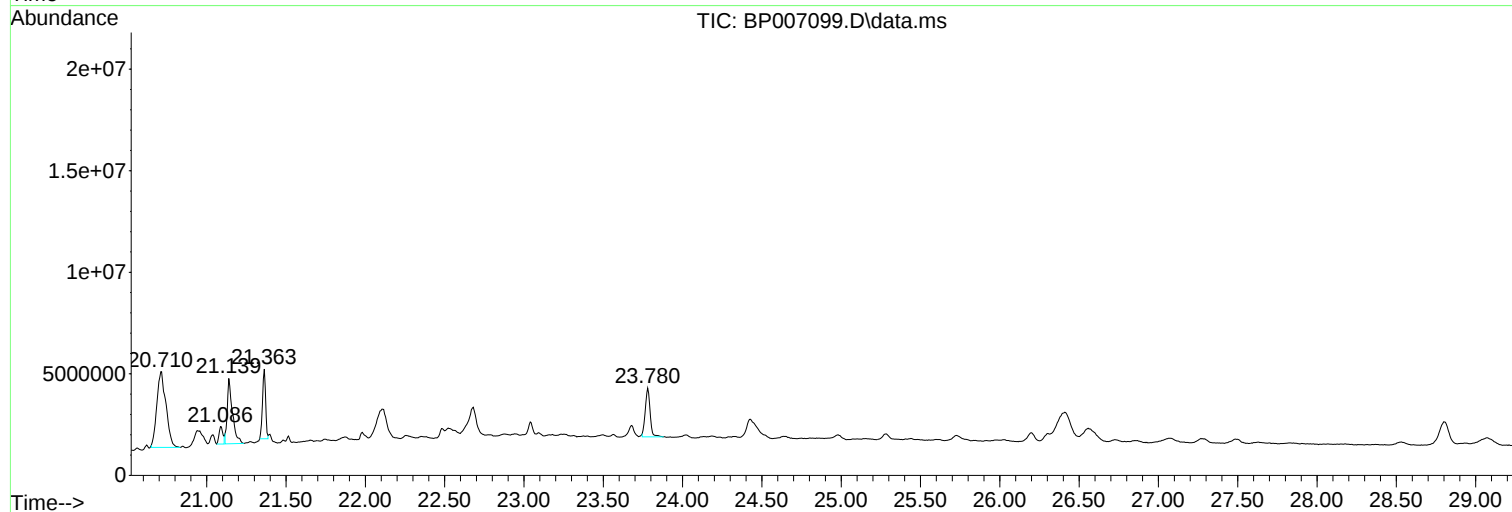
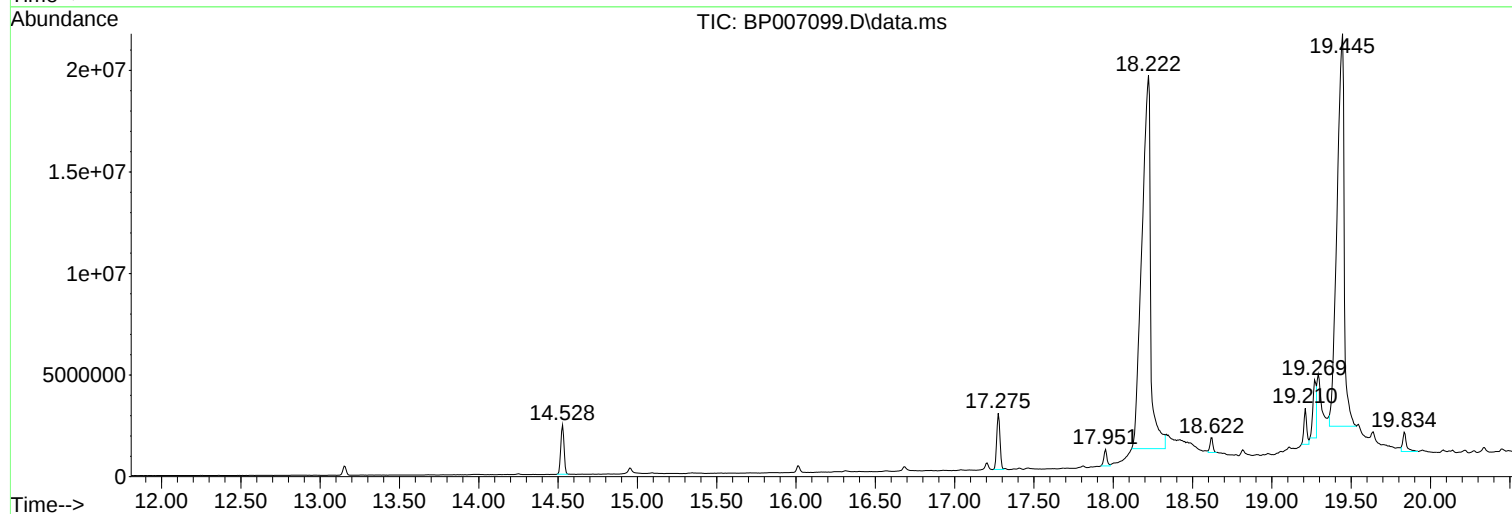
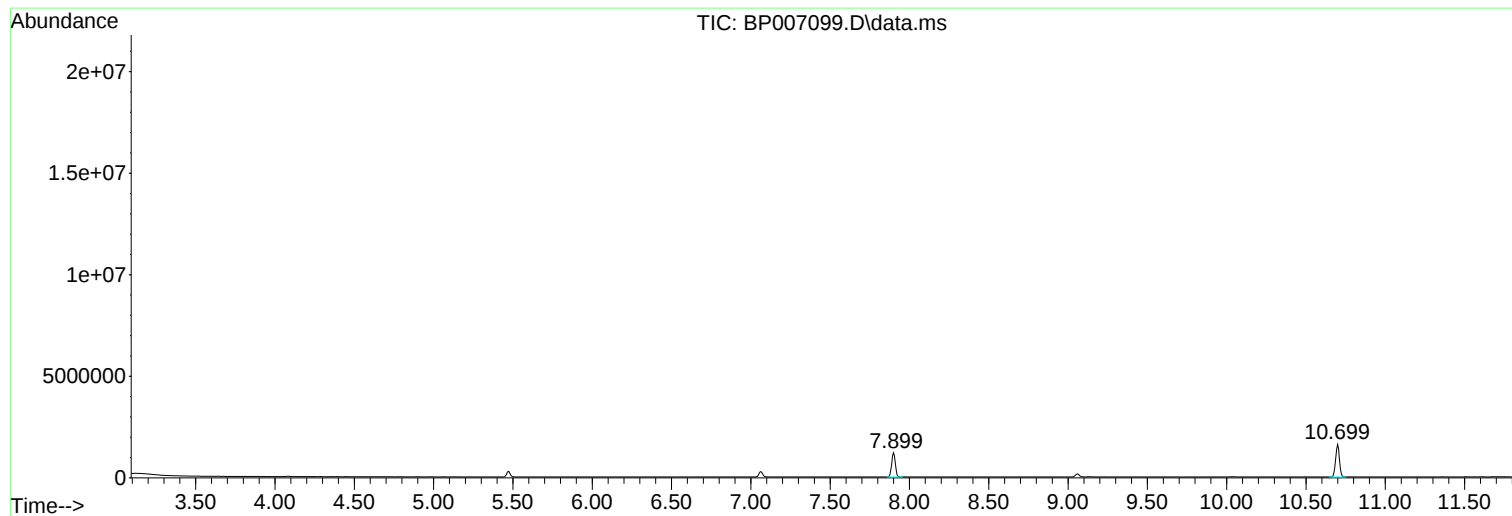
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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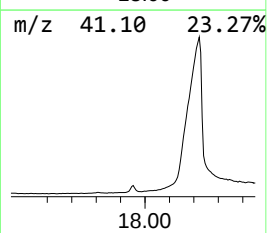
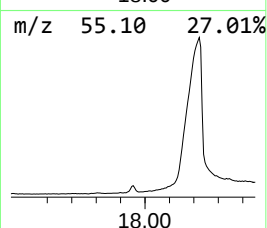
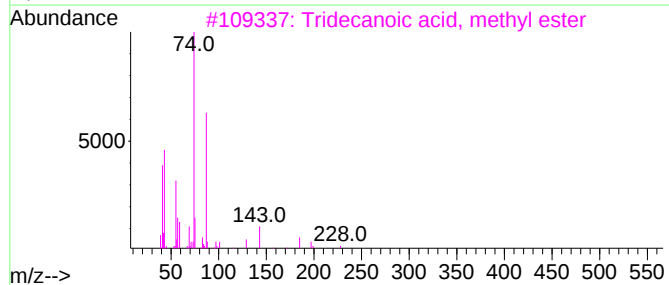
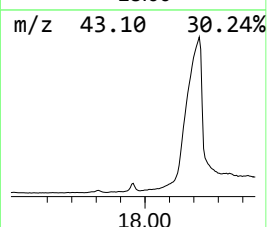
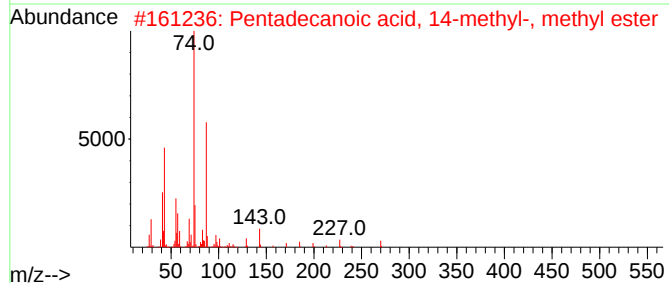
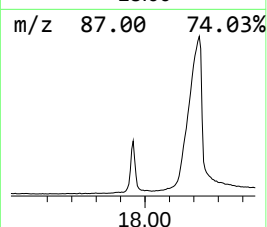
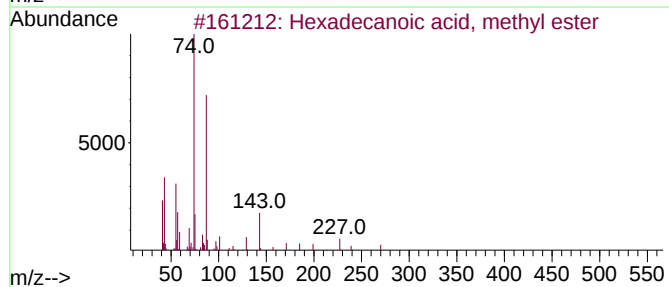
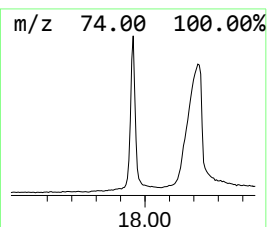
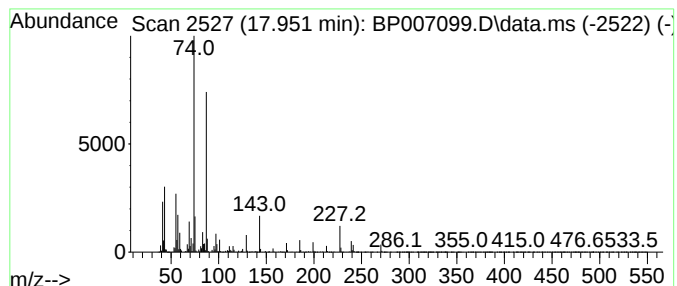
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.951	5.62 ng	1100810	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	91
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	81



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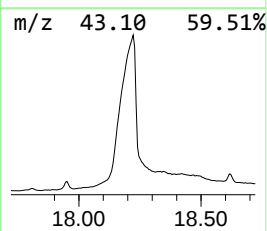
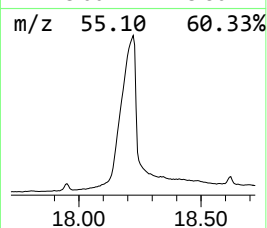
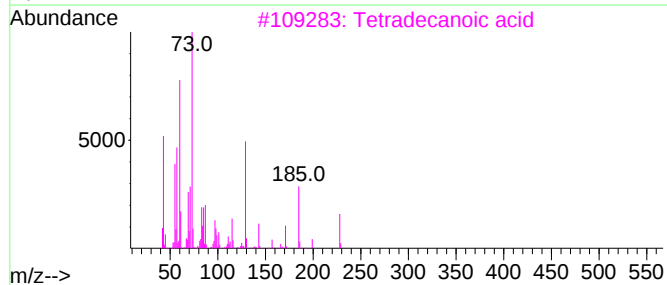
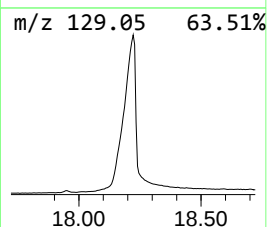
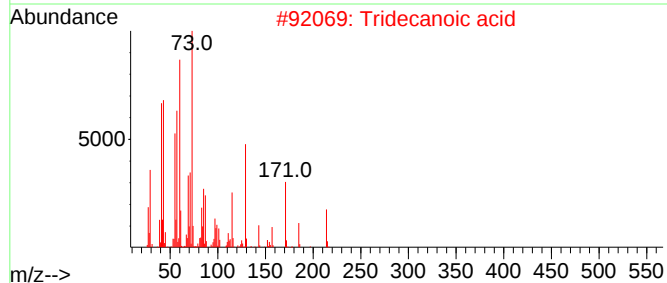
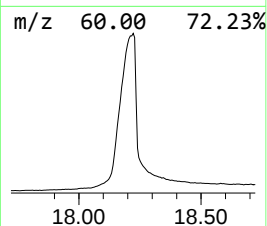
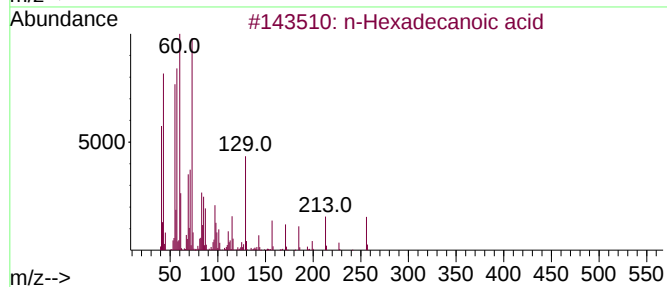
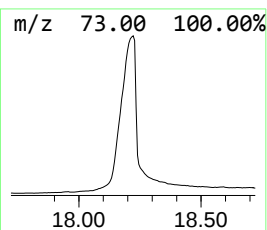
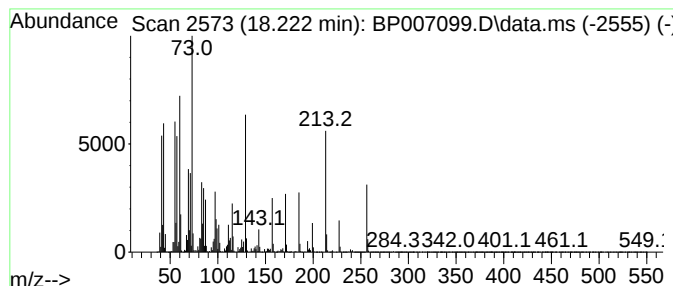
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	362.88 ng	71052700	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5			Octadecanoic acid	284	C18H36O2	000057-11-4	49



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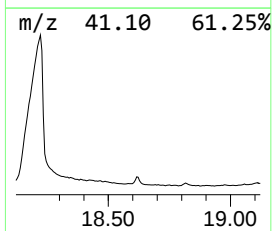
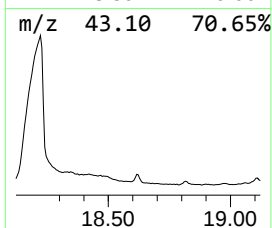
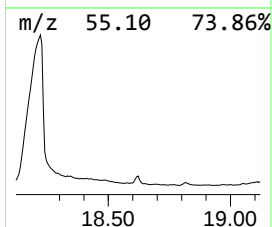
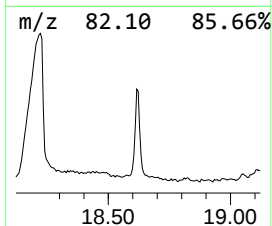
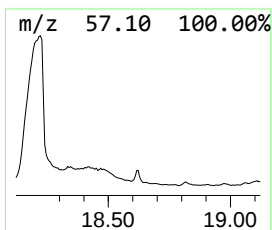
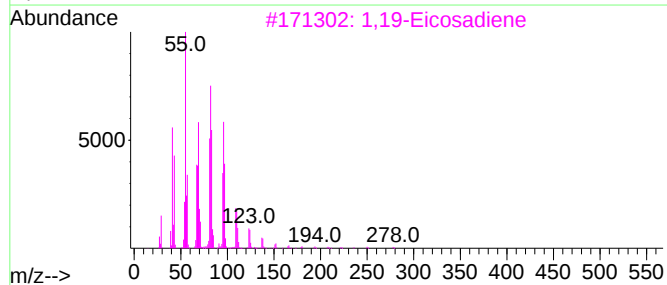
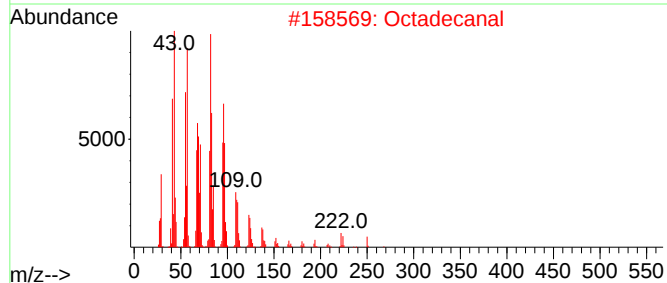
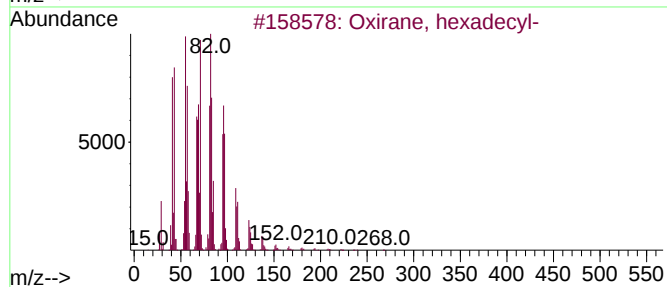
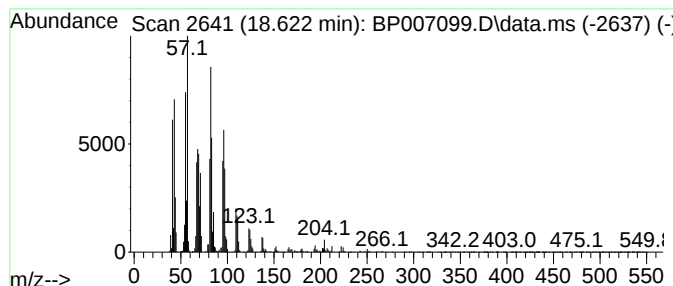
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Peak Number 3 Oxirane, hexadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.622	4.81 ng	941497	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	94
2			Octadecanal	268	C18H36O	000638-66-4	91
3			1,19-Eicosadiene	278	C20H38	014811-95-1	91
4			18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	91
5			Eicosanal-	296	C20H40O	002400-66-0	91



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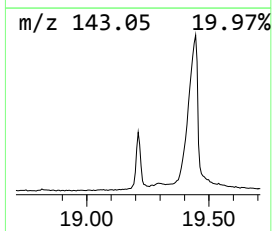
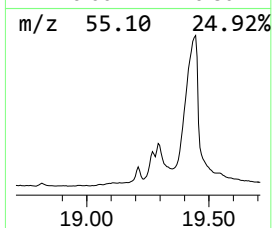
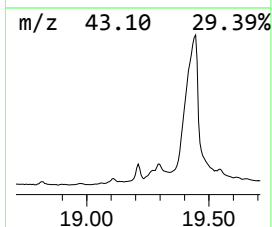
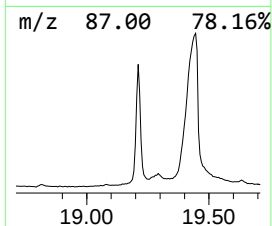
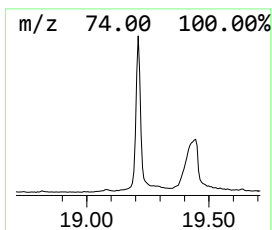
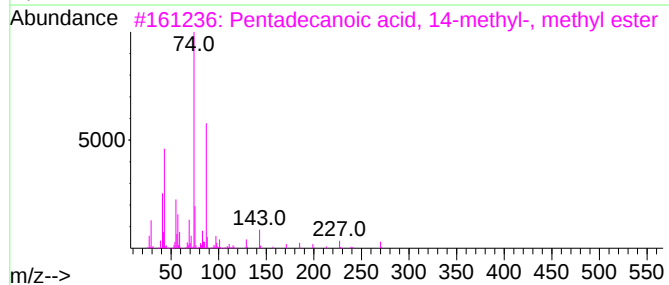
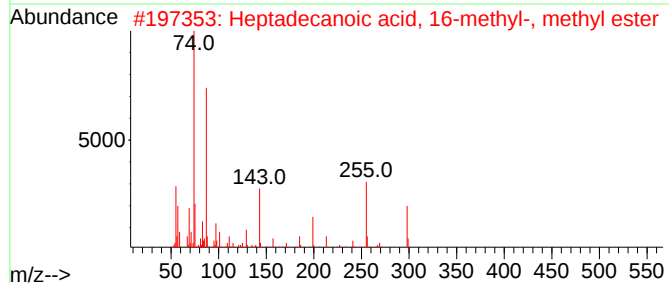
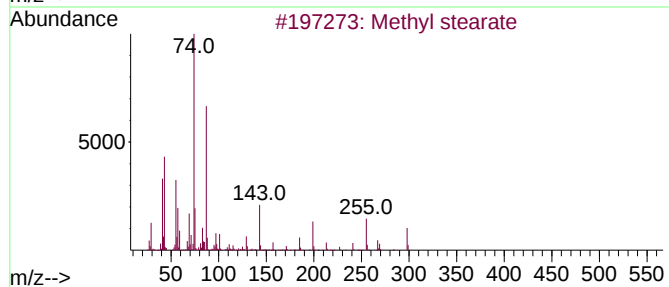
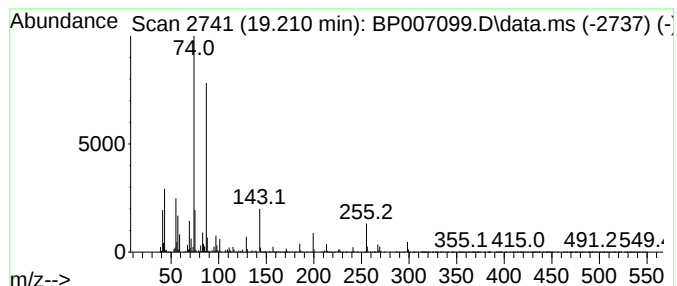
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Peak Number 4 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	11.36 ng	2224220	Phenanthrene-d10	17.275

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	93
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80



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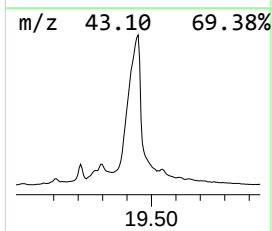
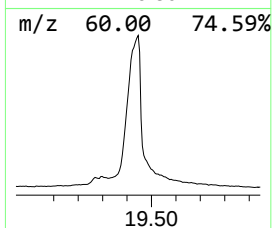
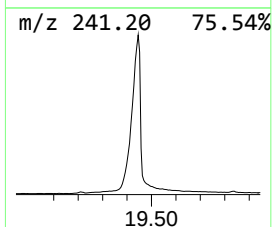
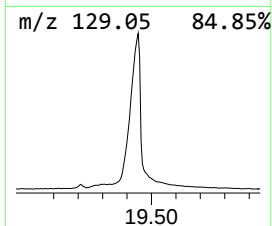
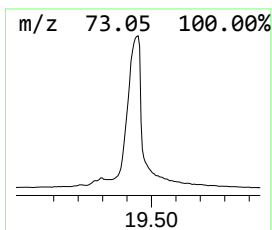
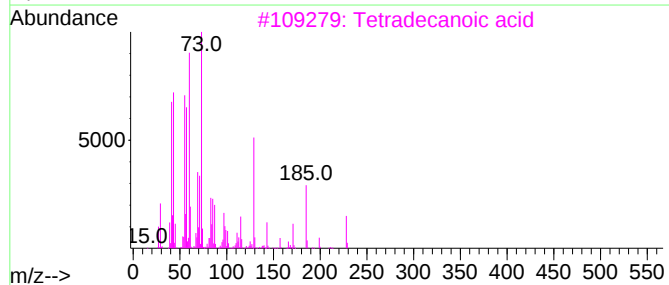
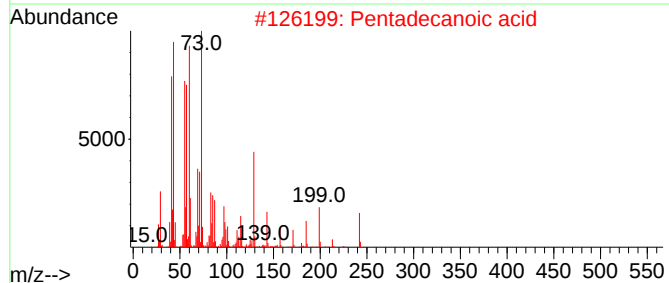
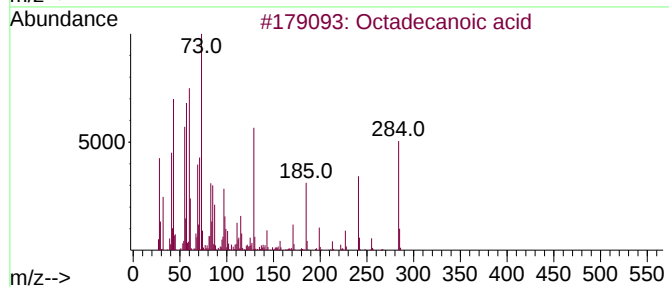
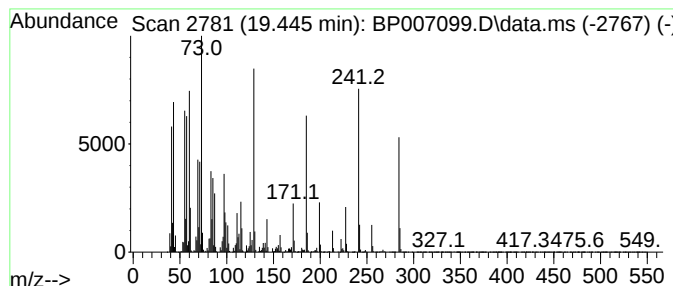
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	261.42 ng	60201900	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	38
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	38



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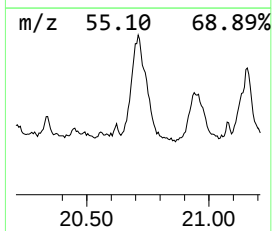
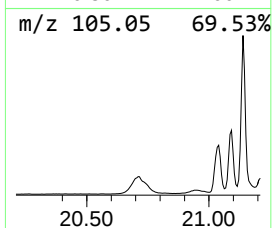
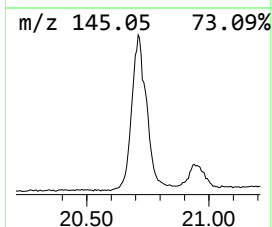
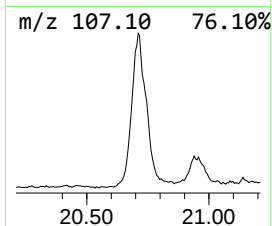
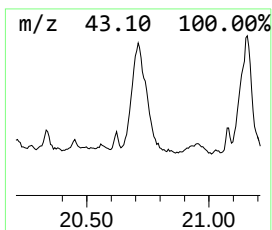
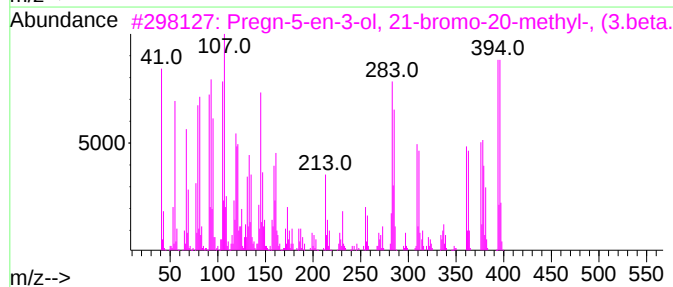
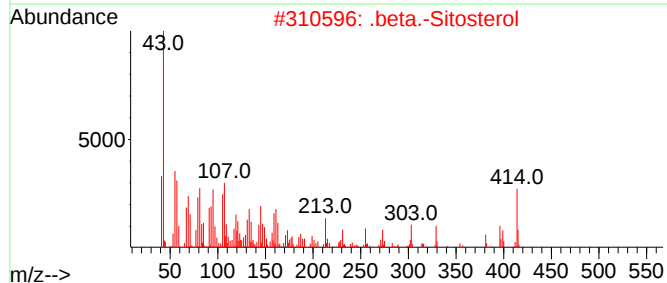
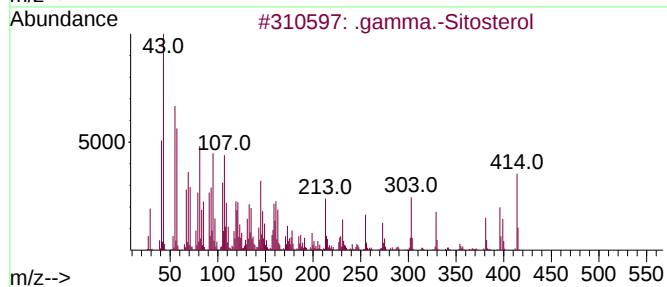
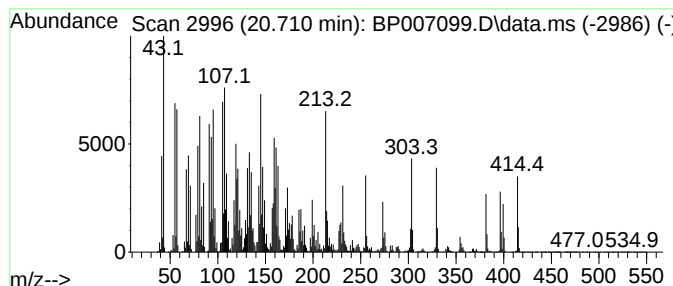
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 .gamma.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.710	64.97 ng	14961900	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-Sitosterol	414	C29H50O	000083-47-6	99	
2	.	beta.-Sitosterol	414	C29H50O	000083-46-5	94	
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	92		
4	(3S,8S,9S,10R,13R,14S,17R)-17-(...	414	C29H50O	029365-29-5	66		
5	17-(1,5-Dimethylhexyl)-10,13-dim...	414	C29H50O	1000210-86-9	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007099.D
Acq On : 22 Sep 2021 15:45
Operator : CG/JU
Sample : M3804-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

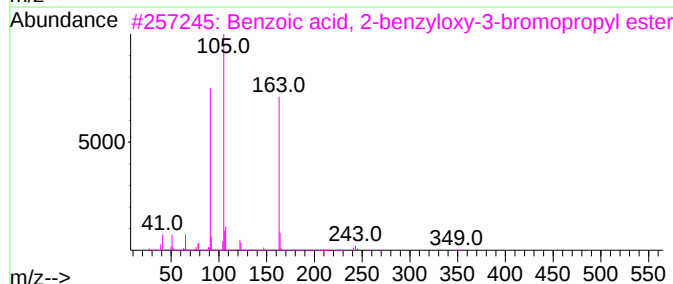
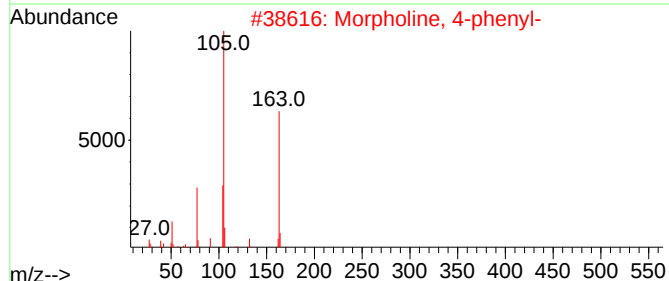
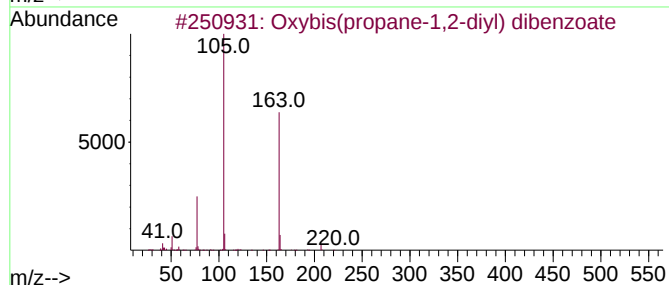
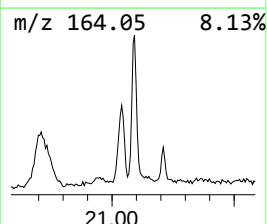
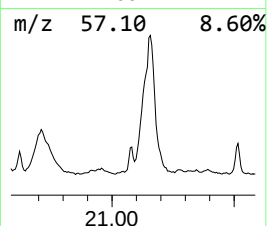
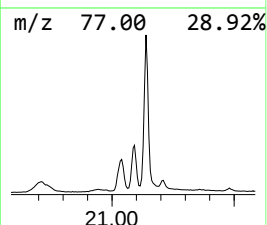
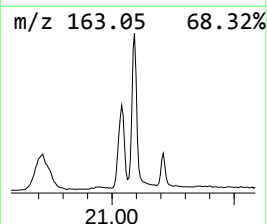
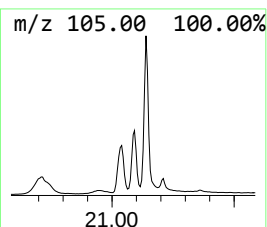
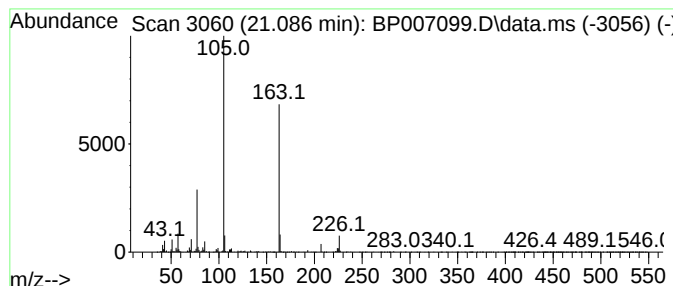
Instrument :
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ClientSampleId :
CL-01-091721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Oxybis(propene-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.086	6.50 ng	1497810	Chrysene-d12	21.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	80
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3	Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	47
4	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
5	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	36



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007099.D
Acq On : 22 Sep 2021 15:45
Operator : CG/JU
Sample : M3804-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CL-01-091721

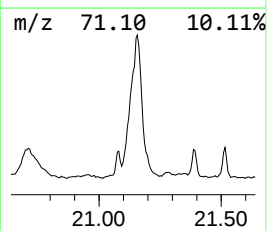
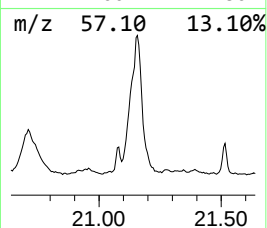
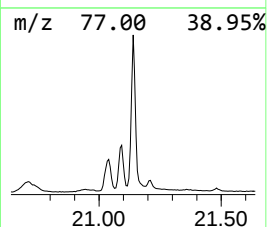
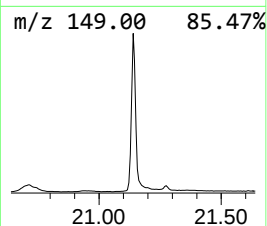
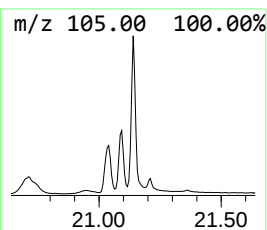
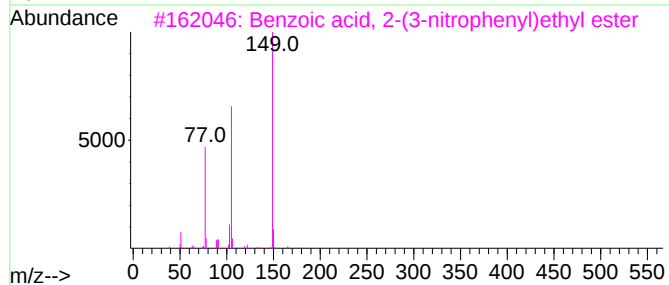
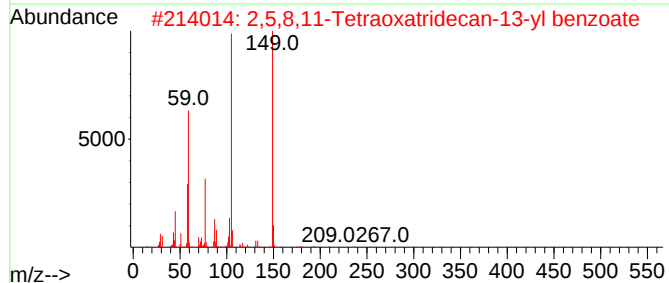
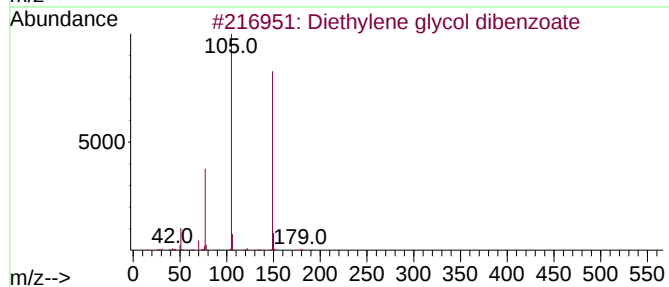
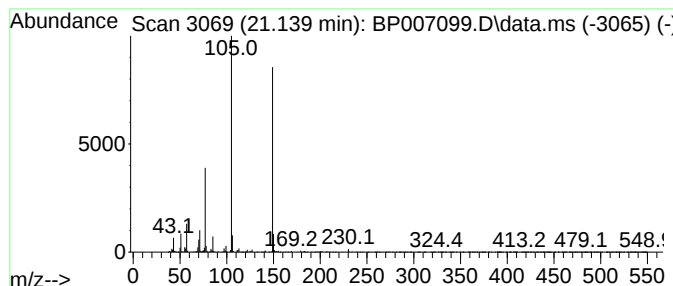
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.139	31.27 ng	7200770	Chrysene-d12	21.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
2			2,5,8,11-Tetraoxatridecan-13-yl ...	312	C16H24O6	1000366-96-7	64
3			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	59
4			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	50
5			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP092221\
Data File : BP007099.D
Acq On : 22 Sep 2021 15:45
Operator : CG/JU
Sample : M3804-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CL-01-091721

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP092121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	17.951	5.6	ng	1100810	4	17.275	3916000	20.0
n-Hexadecanoic ...	18.222	362.9	ng	71052700	4	17.275	3916000	20.0
Oxirane, hexade...	18.622	4.8	ng	941497	4	17.275	3916000	20.0
Methyl stearate	19.210	11.4	ng	2224220	4	17.275	3916000	20.0
Octadecanoic acid	19.445	261.4	ng	60201900	5	21.363	4605810	20.0
.gamma.-Sitosterol	20.710	65.0	ng	14961900	5	21.363	4605810	20.0
Oxybis(propane-...	21.086	6.5	ng	1497810	5	21.363	4605810	20.0
Diethylene glyc...	21.139	31.3	ng	7200770	5	21.363	4605810	20.0